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Temperature dependence of junction voltage in bilayer cuprate superconductors

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Abstract : The present work deals with the study of junction voltage as a function of temperature and various microscopic interactions that exist in bilayer high temperature cuprate superconductors. For this purpose, a tight binding bilayer Hubbard Hamiltonian has been considered that includes the in-plane (within CuO_2 plane) and out-of-plane interactions. The situation for bilayered cuprates considered here is equivalent to a Josephson's coupled SIS junction. We rely on the Green's function equations of motion approach within simple BCS formalism and derive the expressions for superconducting order parameter, carrier density and junction voltage. The numerical analysis shows that in bilayer cuprates, the junction voltage depends on various in-plane and out-of-plane contributions as well as on temperature. Finally, we have compared our theoretical results on junction voltage with that of existing experimental results and found to be in qualitative agreement.

Keywords : Bilayer high-T_c cuprates, Josephson effects, junction voltage.

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1. Introduction

The basic building blocks of the high-T_c cuprate superconductors are the stacks of well-defined two-dimensional CuO_2 planes. For instance, the La_2CuO_4 type of systems have one CuO_2 plane per unit cell while the $YBa_2Cu_3O_{7-x}$ family possess two CuO_2 planes per unit cell and there are other cuprates with still higher number of CuO_2 layers per unit cell.

In $YBa_2Cu_3O_{7-x}$ system, CuO_2 planes are separated by a yttrium ion [1]. Besides this, in YBCO, there are one dimensional CuO chains along b-direction [2]. The CuO_2 planes work as superconducting electrodes separated by BaO, SrO or BiO type of layers which act as weak links or insulating barriers depending on doping. Recently in the superconducting state, the intrinsic Josephson's effect has been discovered in $Bi_2Sr_2CaCu_2O_8$ and later confirmed in $YBa_2Cu_3O_{7-x}$ bilayer system [3–5]. The intrinsic Josephson coupling facilitates the transfer of Cooper pair from one layer to another layer in the superconducting state while in the normal state, the two CuO_2 planes are coupled through single particle tunneling. Therefore, it is interesting to investigate the junction properties like junction voltage, junction resistance, supercurrent *etc* as a function of temperature under competitive Josephson's like Cooper pair and single particle tunneling parameters in these multilayer materials.

The many recent experimental studies also confirm the temperature-dependence of junction voltage in various systems. Very recently, Baselmans *et al* [6] studied the junction voltage $I_c R_n$ product through a superconductor (Nb)-normal metal (Ti-Au bilayer)-superconductor junction as a function of the bath temperature and observed a decrease in the junction voltage with rise in bath temperature. Further, Dubos *et al* [7] performed experiments on Nb-Cu-Nb junctions with highly transparent interfaces and studied the temperature-dependence of eR_nI_c product. They observed a decrease in eR_nI_c product with increase in temperature. Gao *et al* [8] prepared high-T_c Josephson junctions with a graded barrier by using a composite target and studied the effect of temperature on eI_cR_n product. They found that there is a decrease in eI_cR_n product with temperature. They also found enhancement in eI_cR_n product on decreasing the thickness of the graded intermediate layer.

Grant [9] and Hammerl *et al* [10] have shown that at low temperatures, the supercurrent increases substantially by replacing yttrium ion (Y^{3+}) with calcium ion (Ca^{2+}) which is divalent. From temperature-dependence of supercurrent density of these materials, Yurgens *et al* [11] further concluded that the Josephson like junctions are indeed formed within two adjacent CuO_2 layers. Yurgens *et al* [11] studied the hydrostatic pressure-dependence of supercurrent density in $Bi_2Sr_2CaCuO_8$, $Bi_2Sr_{1.5}La_{0.5}CuO_{6-x}$ and $Bi_2Sr_2CaCu_2O_{8+x}$ single crystals. They reported that the supercurrent density increases with the application of hydrostatic pressure and this pressure-dependence of supercurrent density also linked with the possibility of intrinsic Josephson like coupling between the stack of CuO_2 planes in these materials.

Very recently, Singh *et al* [12] studied the temperature-dependence of supercurrent density (I_c) in $YBa_2Cu_3O_{7-x}$ system. They concluded that normalised supercurrent density decreases with normalised temperature and increases, on increasing carrier density within the plane. They, further concluded that the normalised supercurrent density increases on increasing Cooper pair tunneling term.

The above results point towards the importance of the Josephson like coupling between the stack of CuO_2 planes in the superconducting state in a given multilayer cuprate system. The above facts have motivated us to study the junction voltage of these bilayer materials by considering a microscopic tight binding bilayered Hubbard model which includes all possible in-plane and out-of-plane hopping and interaction energies.

2. Theoretical model for bilayer cuprates

We consider the cuprates like $YBa_2Cu_3O_{7-x}$ having two CuO_2 planes per unit cell. As it is believed that the physics of superconducting CuO_2 planes can be well-captured by a two-dimensional tight binding Hubbard model, hence we simulate the coupled CuO_2 planes by a bilayer Hubbard model with an effective attractive interaction within the plane. In order to introduce the coupling between neighbour CuO_2 planes within the unit cell, we will incorporate single particle tunneling as well as Josephson like Cooper pair tunneling terms in the model Hamiltonian and analyse the role of these couplings on the junction voltage. This situation for the bilayered cuprates will just serve as a SIS junction [13] alongwith a sort of Josephson like coupling, where CuO_2 planes are working as superconducting electrodes separated by BaO types of insulating layer. Thus, the microscopic tight binding model Hamiltonian of our bilayer system is given by :

$$H_{\text{bilayer}} = H_{\text{intra}} + H_{\text{inter}}\,, \tag{1}$$

where $$H_{\text{intra}} = -\sum_{rij\sigma}(t_{ij}-\mu)\,C^{+}_{ri\sigma}C_{rj\sigma} + U\sum n_{ri\sigma}\,n_{ri-\sigma}$$
$$+\frac{1}{2}\sum_{ij\sigma\sigma' r} W_{ij} n_{ri\sigma}\, n_{rj\sigma'} \tag{1a}$$

and $$H_{\text{inter}} = \frac{1}{2}\sum_{r\neq s\,ij\sigma}\varepsilon_{K\perp}\left(C^{+}_{ri\sigma}C_{sj\sigma}+h.c\right)$$
$$+Z\sum_{r\neq s\,ij\sigma}\left(C^{+}_{ri\sigma}C^{+}_{ri-\sigma}C_{sj-\sigma}C_{sj\sigma}+h.c\right). \tag{1b}$$

where t_{ij} is the hopping matrix element within the plane and μ is the chemical potential. U and W are on-site and inter-site attractive interactions within CuO_2 plane; r, s are layer indices, with $r = 1(2)$, $s = 2(1)$ for the bilayer systems; i, j are the hole sites; $\sigma(-\sigma)$ are the spin of holes, $C^{+}(C)$ are the creation (annihilation) operator for holes within CuO_2 planes. The H_{intra} part of the model Hamiltonian given by eq. (1a) is just the BCS – Hamiltonian with an effective attractive interaction that comprises the on-site interaction U and inter-site interaction W within CuO_2 planes. In our present attempts, we consider the on-site interaction U to be attractive as we are interested in the physics of superconduting state. However to study the interplay of magnetism and superconductivity, a repulsive U term is important to take care of electron correlations that exist in cuprates.

The first term in the interlayer part of the model Hamiltonian given by eq. (1b) is the single particle hopping between the planes. The second term contains tunneling parameter Z that defines a Josephson like pair-tunneling process between the two adjacent planes in the unit cell

By performing Fourier transformation in the usual way, the model Hamiltonian can be written in the momentum space. Employing the Green's function, many body technique and using standard procedure recently, Ajay *et al* [12,14,15] and Govind *et al* [16,17] have obtained the expression for the superconducting order parameter within the BCS framework for the above model, which is given by

$$\Delta = \frac{-\tilde{U}\Delta}{N}\sum\left[\frac{\tanh(E_{1K}/2K_BT)}{4E_{1K}}+\frac{\tanh(E_{2K}/2K_BT)}{4E_{2K}}\right] \tag{2}$$

where, Δ is the superconducting order parameter and $\tilde{U} = U + W + Z$, is the effective attractive interaction within the plane. Here, Z is also negative (attractive nature) so that the effective interaction $\tilde{U}$ is assumed to be attractive (negative) to give rise to the pairing within the CuO_2 planes. In the above,

$$E_{1,2K} = \left(\varepsilon^2_{1,2K} + \Delta^2\right)^{1/2};$$

$$\varepsilon_{1,2K} = \left(\varepsilon_K - \mu + (U+W)\langle n_{ab}\rangle\right) \pm \varepsilon_{K\perp};$$

$$\varepsilon_K = -2t_{11}\left(\cos k_x a + \cos k_y a\right);$$

$$\varepsilon_{K\perp} = -2t_\perp \cos k_z a;$$

where, $\langle n_{ab}\rangle$ is the carrier density within the plane in the superconducting state. We have assumed that $\langle n_{ab}\rangle = \langle n_\uparrow\rangle = \langle n_\downarrow\rangle$ and 'a' is lattice parameter. The carrier density $\langle n_{ab}\rangle$ is given as [17] :

$$\langle n_{ab}\rangle = \frac{1}{N}\sum_K \left(\langle\langle C^+_{1K} C_{1K}\rangle\rangle\right) = -\frac{1}{N}\sum_K\left[\frac{\varepsilon_{1K}\tanh(E_{1K}/2K_BT)}{4E_{1K}} \quad \frac{\varepsilon_{2K}\tanh(E_{2K}/2K_BT)}{4E_{2K}}\right] \tag{3}$$

In order to analyse the full temperature-dependence of junction voltage for coupled bilayered system which is equivalent to a SIS junction, we shall use the Ambegaokar-Baratoff microscopic result for a tunnel junction (SIS) [18,19] which is given by

$$I_c R_n = \frac{\pi\Delta(T)}{2e}\tanh\left\{\frac{\Delta(T)}{2K_BT}\right. \tag{4}$$

where I_c is supercurrent density, R_n is the junction resistance in normal state and I_cR_n is the junction voltage. $\Delta(T)$ is the superconducting order parameter at T ($< T_c$) which is given by eq. (2).

Using eqs. (2) and (4), one can study the junction voltage as a function of temperature and various microscopic parameters of the model Hamiltonian given by eq. (1). A close examination of eqs. (2), (3) and (4), reveal that these are coupled integral equations and require a self-consistent numerical computation.

3. Results and discussion

For the study of junction voltage as a function of temperature and other parameters of the model Hamiltonian of bilayered system considered here, we convert summation over k-values in eq. (2) into an integration and perform numerical calculations self-consistently.

During the numerical calculation, we have taken n_{ab} = 0.085, t_{11} = 200 meV, $t_\perp$ = 20 meV, $\tilde{U}$ = −600 meV [17,20]. The values of superconducting order parameter $\Delta(T)$ have been calculated numerically (self-consistent method) from eq. (2) as a function of temperature and the parameters of the model Hamiltonian. Using these results, finally from eq. (4), we have plotted junction voltage I_cR_n as a function of normalized temperature T/T_c for different values of the model Hamiltonian parameters.

In Figure 1, we have analysed I_cR_n vs T/T_c for different values of carrier density in the plane ($\langle n_{ab}\rangle$). From Figure 1,

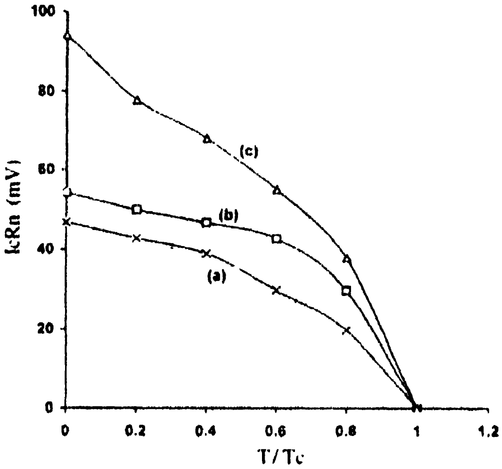

Figure 1. The variation of I_cR_n vs T/T_c with (a) n_{ab} = 0.085 (cross) (b) n_{ab} = 0.095 (square), (c) n_{ab} = 0.105 (triangle). The other parameters are t_{11} = 200 meV, $t_\perp$ = 20 meV, $\tilde{U}$ = −600 meV

it is clear that on increasing carrier density in the plane from (a) n_{ab} = 0.085 to (c) n_{ab} = 0.105, the junction voltage increases and its rate with normalized temperature decreases less rapidly. This slowly decreasing rate of I_cR_n with T/T_c on increasing n_{ab} is a consequence of increase in superconducting order parameter with n_{ab} from under-doped to optimal-doped condition in cuprates [12,16,17].

In Figure 2, the variation of I_cR_n vs T/T_c has been plotted for different values of Josephson like Cooper pair tunneling

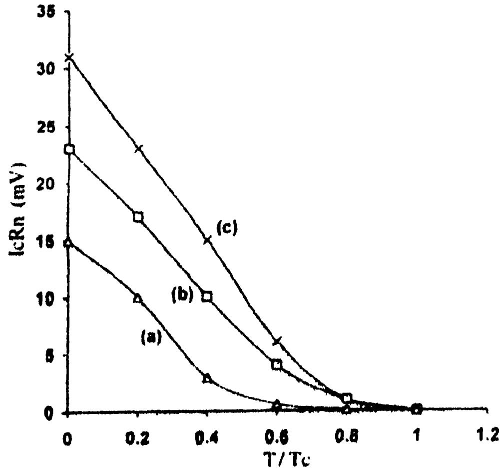

Figure 2. The variation of I_cR_n vs T/T_c with (a) in the absence of pair tunneling *i.e.* $Z \to 0$ (triangle), (b) Z = −40 meV (square), (c) Z = −70 meV (cross). The other parameters are n_{ab} = 0.085, t_{11} = 200 meV, $t_\perp$ = 20 meV; keeping $U + W$ = −600 meV.

term (Z) : (a) $Z = 0$, (b) $Z = -40$ meV, (c) $Z = -70$ meV and keeping all other parameters fixed ($n_{ab} = 0.085$, $t_{\parallel} = 200$ meV, $t_{\perp} = 20$ meV, $U + W = -600$ meV). It can be seen from Figure 2 that on increasing Z, the junction voltage increases and the rate at which I_cR_n decreases with T/T_c becomes low. This implies that Josephson coupling between the layers of a bilayer cuprate system enhances the junction voltage. This increase in I_cR_n on increasing Josephson coupling strength between the layers is through increase in superconducting order parameter [12,14–17].

The numerical results of enhancement of junction voltage on increasing carrier density [as shown in Figure 1] can also be connected with the experimentally observed increment in supercurrent density with doping of Ca^{2+} ion in place of Y^{3+} ion. As Y^{3+} ion is located within the insulating interface between the two CuO_2 planes within the unit cell in $YBa_2Cu_3O_{7-\delta}$ system and replacement of a Y^{3+} ion with Ca^{2+} ion will introduce a hole at the insulating interface which further enhances the coupling between the planes and thereby enhancement in the supercurrent density and hence enhancement in the junction voltage (since below T_c, I_cR_n product has the same trend as I_c with temperature). These observations are in qualitative agreement with the experimental results of Hammerl *et al* [10].

We can also compare the results of the variation of I_cR_n *vs* T/T_c shown in Figure 2 for different values of Josephson coupling term (Z) with that of the recent experimental results of Yurgens *et al* [11] on temperature-dependence of the supercurrent density at different hydrostatic pressure. These authors found that supercurrent density increases substantially with pressure at all temperatures below T_c. In our present tight binding model calculation within simple BCS formalism on increasing pressure in the superconducting state, the transfer of Cooper pairs from one layer to another may also increase and thereby Josephson's coupling between the superconducting plane (Z) increases and gives rise to an increase in supercurrent density and thereby junction voltage as shown in Figure 2, which is in qualitative agreement with the experimental observation [11]. Hence, Josephson like interlayer coupling have pronounce effect on junction voltage in multilayered superconducting system.

4. Conclusions

Finally, we have shown using tight binding bilayer Hubbard model within simple BCS formalism that the normalized junction voltage depend on various microscopic couplings and interactions within and between CuO_2 planes as well as on temperature in an essential way. Our theoretical results on junction voltage are in qualitative agreement with the recent experimental results where enhancement of supercurrent density with pressure as well as chemical substitution of Ca^{2+} ion in place of Y^{3+} ion is observed in YBCO [10].

In the present study, we have considered mainly the temperature dependence of junction voltage. It will be interesting to extend the present tight binding calculation by incorporating the magnetic field in multilayer cuprate systems.

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